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Multiscale mechanical behavior and microstructure evolution of extruded magnesium alloy sheets: Experimental and crystal plasticity analysis

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ABSTRACT

A phenomenological crystal plasticity finite element (CPFE) model based on Voronoi grains was applied to reproduce basic deformation features of a hot-extruded magnesium alloy sheet under various strain paths. Corresponding experimental investigations, including mechanical tests, electron back scattered diffraction (EBSD) measurements and optical observation, were also carried out as either a validation or a supplement of the numerical results. Predicted average stress-strain responses and texture evolution are in good accordance with measured ones. Furthermore, deformation heterogeneity at the mesoscopic and intergranular scale were investigated based on the proposed model. At the mesoscale, the heterogeneity in the slip-dominated cases tends to develop continuously, whereas the heterogeneity is retarded in twin-favored deformation. At the intergranular scale, it is concluded from the slip-dominated case that a high slip-transfer parameter and high Schmid factors (SFs) of principal slip systems in adjacent grains could accommodate higher local strain.

1. Introduction

Magnesium alloys have great potential in automotive industries due to relatively high specific strength [1], and in biomedical implants due to attractive biocompatibility [2]. However, the applications of wrought magnesium alloys as structural components are considerably hindered due to low ductility and strong deformation anisotropy at room temperature (RT). Such deficiencies can be overcome by alloying with proper elements, such as rare-earth elements, altering intrinsic deformation mechanisms and subsequent texture evolution [3]. Thus, a sound understanding of deformation mechanisms and their impact on mechanical properties and texture evolution is required as a prerequisite for Mg alloys used in structural applications.

Due to the hexagonal closed packed (HCP) crystal structure, the main deformation modes in magnesium alloys include: basal ⟨a⟩ slip, prismatic ⟨a⟩ slip, pyramidal ⟨a⟩ slip, pyramidal ⟨c + a⟩ slip, tension twin and compression twin. Different loading conditions result in discrepant dominant modes and resultant textures. As reported, pyramidal ⟨c + a⟩ and basal ⟨a⟩ slip dominate the deformation in magnesium alloy sheets under through-thickness compression, leading to a stronger basal texture [4]. Tension twinning, accompanied with twin-induced reorientation is more favored in sheets during in-plane compression [5]. Furthermore, various dominant modes also lead to a discrepancy in heterogeneous deformation. At the microscopic scale, Sun et al. [6] studied a grain-scale deformation using in-situ tension in scanning electron microscopy (SEM) combined with electron back scattered diffraction (EBSD) and digital image correlation (DIC) techniques. It is concluded that both the slip-transfer parameter in the grain boundary and the Schmid factor (SF) of certain slip system in the adjacent grains influence the ability in accommodating microscopic deformation. At the mesoscopic scale, Lu et al. [7] investigated anisotropic deformation of extruded AZ31 rods under uniaxial compression using in-situ synchrotron X-ray imaging and diffraction. The profuse activity of tension twin is found resulting reduced strain localization, while the dominance of dislocation slip leads to obvious non-uniform deformation. At the macroscopic scale, Hazeli et al. [8] used DIC and acoustic emission to investigate the near-yielding behavior of AZ31 rolled sheet. Tension twin is found to be closely related to strain localization in the form of apparent bands near yielding under in-plane compression. Kapan et al. [9] also investigated macro strain heterogeneity in rolled and extruded AZ31 samples. Sharper banding structures were observed in rolled samples than extruded ones.

Apart from experimental investigations, numerical simulations are also carried out to study the deformation of magnesium alloy. Crystal

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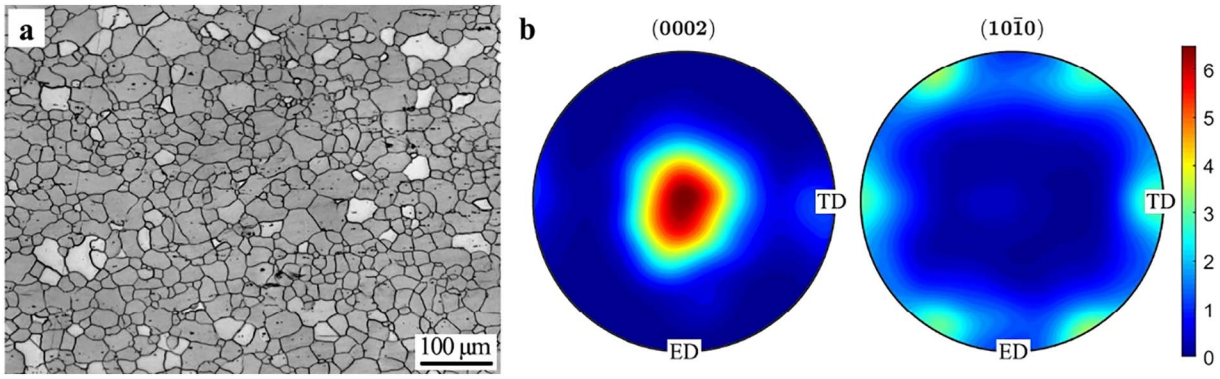

Fig. 1. Initial state of magnesium alloy extruded sheet after annealing: (a) optical micrograph; (b) pole figures (PFs) from calculated average ODF. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

plasticity (CP) models, which explicitly describe the deformation modes, have been proved an appropriate approach for studying crystalline materials at macro-and microscopic scale. At the constitutive level for single crystals, deformation twinning is typically treated as a pseudo-slip [10], and twin-induced reorientation effect is considered in various ways: (i) the predominant twin reorientation (PTR) method [10]; (ii) the volume fraction transfer (VFT) scheme [11]; (iii) the total Lagrangian approach [12]; (iv) the composite grain (CG) method [13]; (iv) the twinning-detwinning (TDT) model [14]. Latent hardening (LH) due to slip-slip, slip-twin and twin-twin interactions is another key point in CP models, especially for HCP metals. Recently, Bhattacharyya et al. [15] considered LH of slip modes based on a discrete dislocation dynamics study [16], while the rest of CP-based simulations tend to decide LH coefficients by parameter fitting empirically. Furthermore, the relationship between the deformation of the single crystal and that of the polycrystalline aggregate is now calculated in either mean-field models, such as Taylor models [17] and self-consistent (SC) models [18], or spatial CP models, such as CP based finite element (CPFE) models [19] and CP based fast Fourier transformation (CPFFT) models [20]. Both types of models (mean-field and spatial CP) have been successfully applied for the analysis of stress-strain response, slip/twin activity and deformation texture in magnesium alloys [14,15,21,22], while spatial CP models account for grain-to-grain interactions and thus have more flexibility in calculating inhomogeneous fields. Prakash et al. [23] investigated the evolution of grain shape as well as localized shear region using CPFE models. Based on CPFFT modeling, Sinclair et al. [24] reported that higher anisotropy in slip system strength and weaker texture intensity would increase heterogeneity. Despite several experimental studies carried out on inhomogeneous deformation in magnesium alloys, the corresponding numerical study is relatively limited. Deformation heterogeneity is understood to be a precursor to damage nucleation [25], thus such a topic deserves a comprehensive investigation.

In the present work, a phenomenological CPFE model based on Voronoi grains was applied to simulate the deformations of a hot-extruded magnesium alloy sheet under various strain paths. Combined with experimental measurements, average mechanical behavior and texture evolution were examined first. Then, deformation heterogeneity at the mesoscopic scale and intergranular scale were investigated and discussed based on the proposed model.

2. Experimental and Numerical Setup

2.1. Experimental Procedures

The material studied in this work was a hot-extruded magnesium alloy (3.9% Al, 1.0% Zn, 0.4% Mn, Balanced Mg in wt%) sheet with 6 mm thickness. The sheets, wrapped with aluminum foil to minimize oxidation, were then annealed at 450 °C for 3 h and air cooled to room temperature. Sub-size (Scale-down) dog-bone tension samples according to ASTM-E8 standard were prepared for uniaxial tensile tests along ED (extrusion direction). Brick samples with dimensions of 9 × 6 × 6 mm and 6 × 4 × 4 mm were prepared for uniaxial compression tests along ED and ND (normal or through-thickness direction), respectively. Tensile tests were carried out on a universal material tester (Shimadzu, AG-X) machine, while compression tests using a thermal and mechanical testing system (Gleeble 1500D). All tests were at an initial strain rate of 0.001 s^{-1} and room temperature. In the following description, the samples are named with ED-t, ED-c and ND-c ('c' or 't' for compression or tension, respectively). Under each deformation condition, three samples were tested to rupture, and one more sample was interrupted at specific plastic strain for metallographic and texture examination.

The undeformed and deformed samples were first ground by abrasive papers up to 4000 grit, then polished using 1 μm diamond suspension and finally polished with OP-S (colloidal silica) solution. EBSD measurements were carried out using Auger Electron Spectroscopy (PHI 710) with an EDAX-TSL system. The texture was measured on maps of 250 × 250 μm with a step size of 0.8 μm. TSL OIM analysis 7.3 software and Matlab toolbox MTEX 4.5 [26] were used for the analysis of EBSD data. For the initial texture, three EBSD maps were adopted to calculate an average orientation distribution function (ODF) and pole figures, which were subsequently used for the input of the simulation. The samples were further etched in a solution of 6 g picric acid, 10 ml acetic acid, 10 ml H_2O and 100 ml ethanol for about 15 s for optical microstructure examination. All the examinations were carried out on the ED × TD (TD for transverse direction) plane. The initial microstructure and texture are shown in Fig. 1, which indicate equiaxed grains and a nearly basal texture.

2.2. Modeling Framework

A phenomenological CP constitutive model was employed to model plastic deformation based on various deformation mechanisms, which included basal ⟨a⟩ slip ({0001} ⟨11$\bar{2}$0⟩), prismatic ⟨a⟩ slip ({10$\bar{1}$0} ⟨11$\bar{2}$0⟩), pyramidal ⟨c + a⟩ slip ({11$\bar{2}$2} ⟨11$\bar{2}$3⟩) and tension twin ({10$\bar{1}$2} ⟨10$\bar{1}$1⟩). Notably, compression twin was not considered in the present work, for the reason that compression twin was reported to have more influence on fracture than ductility [27]. A brief description of the formulations is given here, while a detailed version can be found in our previous work [28].

The plastic velocity gradient is expressed as [12]: